Heat Conduction by Molecular Dynamics Technique

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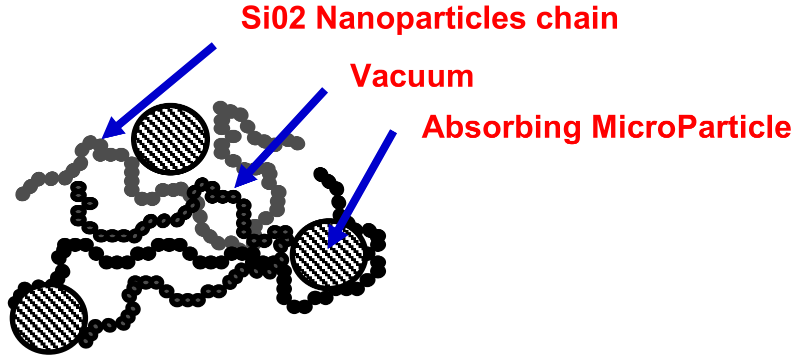
UNDERSTANDING AND MONITORING MATERIALS PROPERTIES

NEW MATERIALS contain nano-micro architectured structures

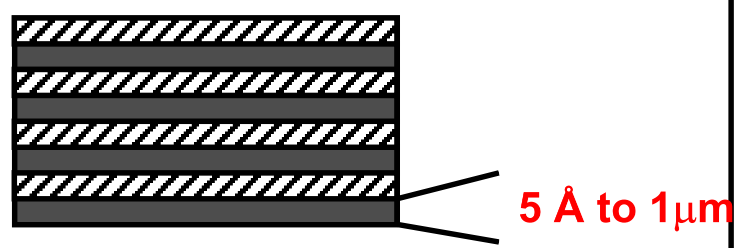
o NANOFIBERS:

multiscale complex materials
***ultra insulating* (0.007 W/mK)**



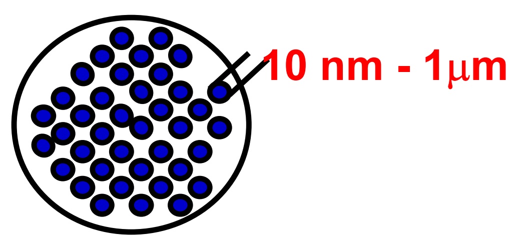
o SUPERLATTICES

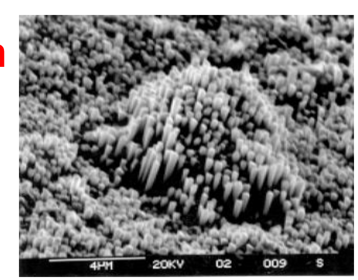
monitoring thermal conductivity
$\lambda_{Bulk}/10<\lambda<\lambda_{Bulk}$



o NANOWIRES templates:

monitoring anisotropy

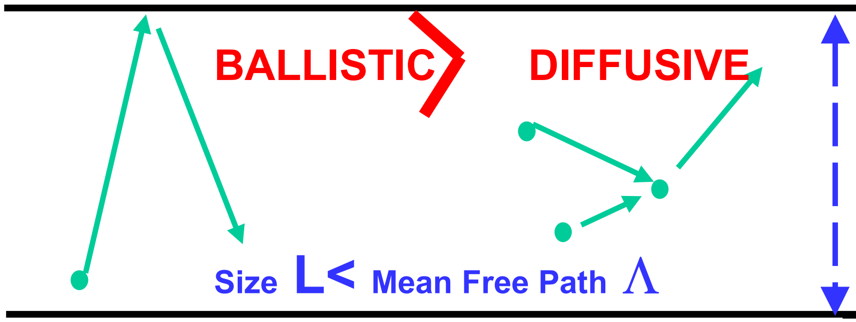




G. Chen - Ni nanowires template

LOW-DIMENSIONAL PHYSICS FOR HEAT CONDUCTION

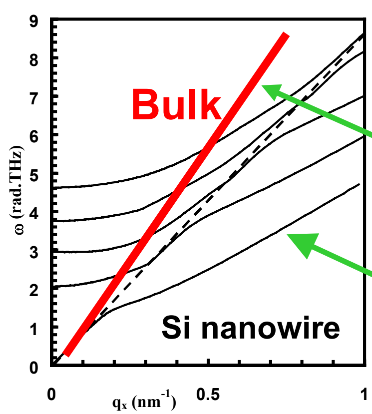
o Ballistic Transport of Phonons



Boundary Scattering
More resistive

o Phonon Confinement

v_G and Λ Reduction



$$\frac{\partial^2 u}{\partial t^2} = v_t^2 . \nabla^2 u + \left(v_l^2 - v_t^2\right) \nabla (\nabla \bullet u)$$

$$\cancel{\vec{q} = -\lambda_{BULK} . \overrightarrow{grad\ T}}$$

$$\lambda_{eff}(\text{size}) < \lambda_{BULK}$$

SITUATION of MD

Small Scales

Phonon Transport: Ballistic → Diffusive

Phonon Particle: Boltzmann TE
No interference, Interface transfer
Small and Large scales

Phonon Wave
No p-p scattering, limited by wl
Interface transfer easier

Molecular Dynamics - MD

Classical Heat Conduction

$$\vec{q} = -\lambda_{BULK} \cdot \overrightarrow{grad}\, T$$

Atomic Period 0.1ps
Lattice Constant 0.5nm

Relaxation time 100ps
Mean Free Path 100nm

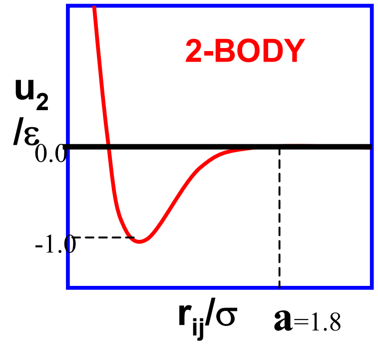
MOLECULAR DYNAMICS TECHNIQUE

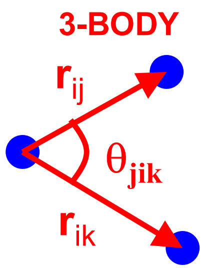
COMPUTE ALL ATOMIC TRAJECTORIES

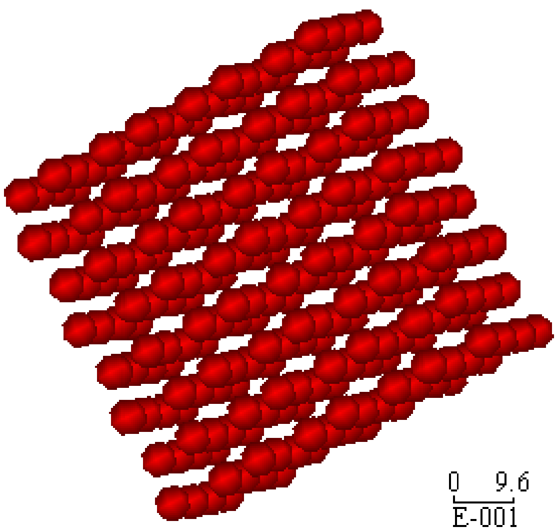
- **2nd NEWTON LAW**

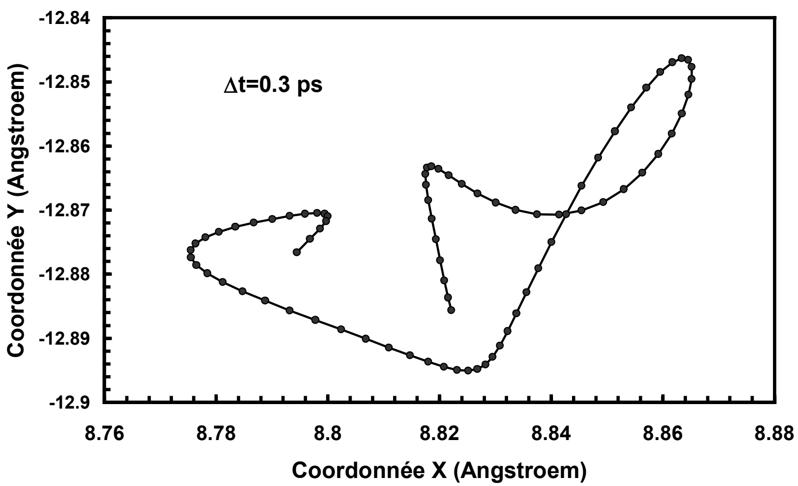
$$M \frac{d^2 \mathbf{r}_i}{dt^2} = \sum_{\substack{j=1 \\ j \neq i}}^{N} \mathbf{F}_{ij}$$

- **STILLINGER-WEBER POTENTIAL**









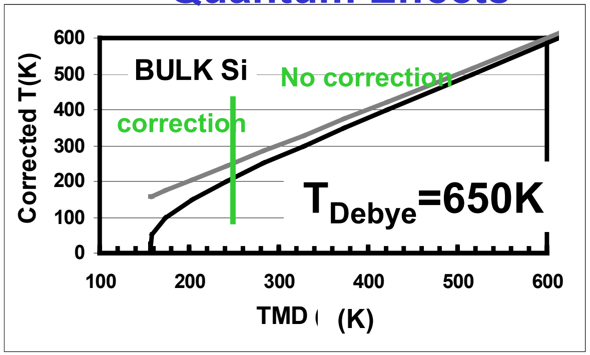
ADVANTAGES OF MD TECHNIQUE

o **Phonon Scattering is Difficult to Model:**
Phonon Particle Approach: Relaxation Time ??
Phonon Wave Approach: No scattering.

MD PROVIDES A COMPLETE DESCRIPTION OF PHONON SCATTERING

EXAMPLE: NANOWIRE

Quantum Effects



o **Phonon Transport Approach Assumes Fully Periodic Lattices**

MD ALLOWS TO INCLUDE ATOMIC DEFAULTS and STRAINS

EXAMPLE: SUPERLATTICE

o **Non-Equilibrium Short Time Heat Conduction**

MD DESCRIBE HT BEHAVIOUR AT GigaHTz FREQUENCIES

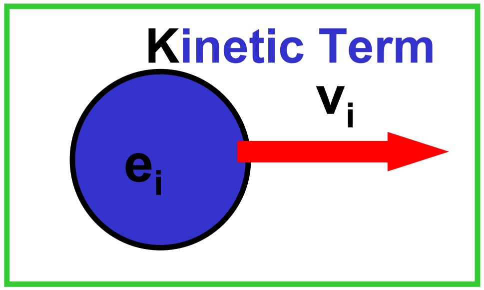
EXAMPLE: IN BULK SI

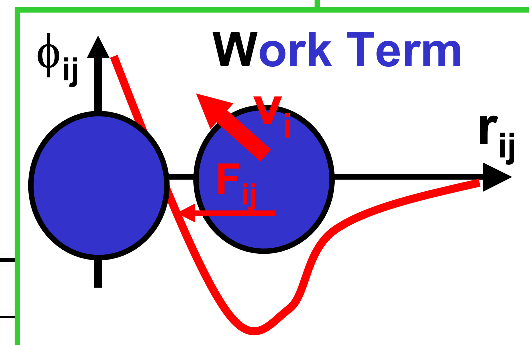
HEAT FLUX by MD

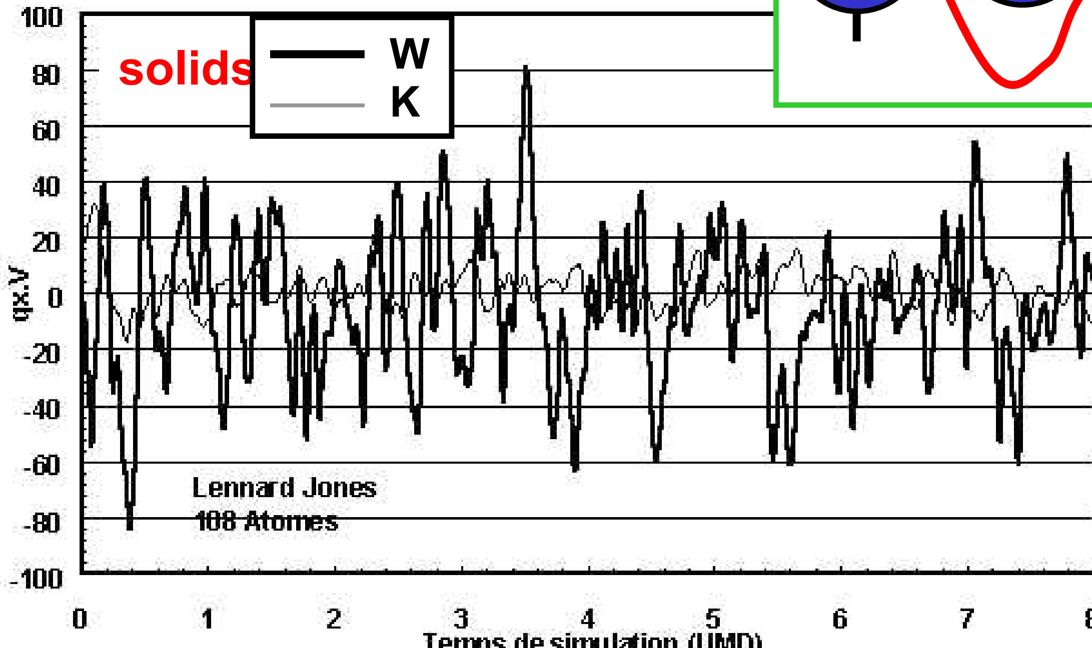
o Kinetic and Work terms

solids

$$\mathbf{q}_0(t) = \frac{1}{V}\left[\cancel{\sum_{i=1}^{N} e_i \mathbf{v}_i} - \frac{1}{2}\sum_{\substack{j=1 \\ j\neq i}}^{N}\left(\mathbf{v}_i . \left(\overleftrightarrow{\mathbf{F}_{ij} . \mathbf{r}_{ij}}\right)\right)\right]$$







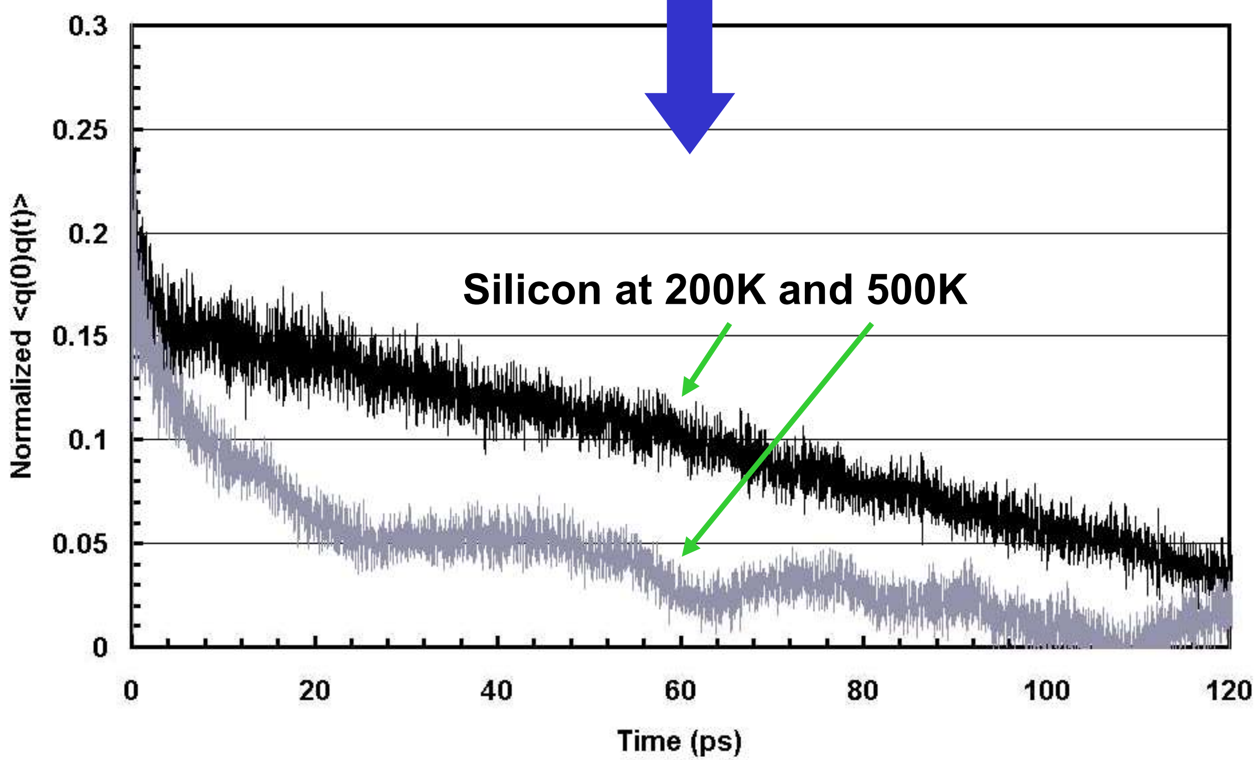
THERMAL CONDUCTIVITY by MD

ω=0, Thermal Conductivity

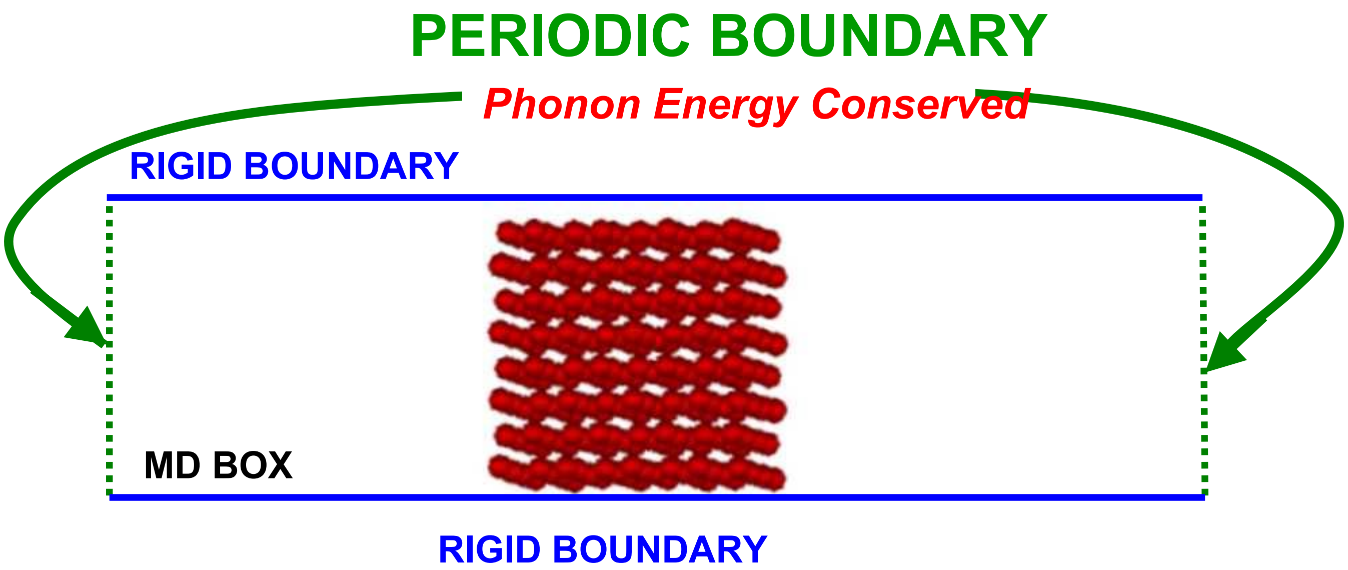
o **Fluctuation-Dissipation Theorem**

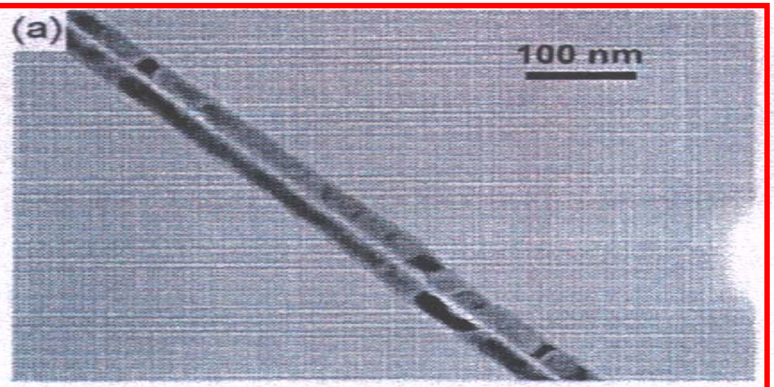
gradT X $\lambda(\omega) = \dfrac{V}{3k_B T_0^{\;2}} \int_0^{\infty} \langle \mathbf{q}_0(0)\mathbf{q}_0(\tau)\rangle e^{i\omega\tau}\, d\tau$ X **grad**T

The Flux **Autocorrelation** **The Force**



SILICON NANOWIRE MD MODEL

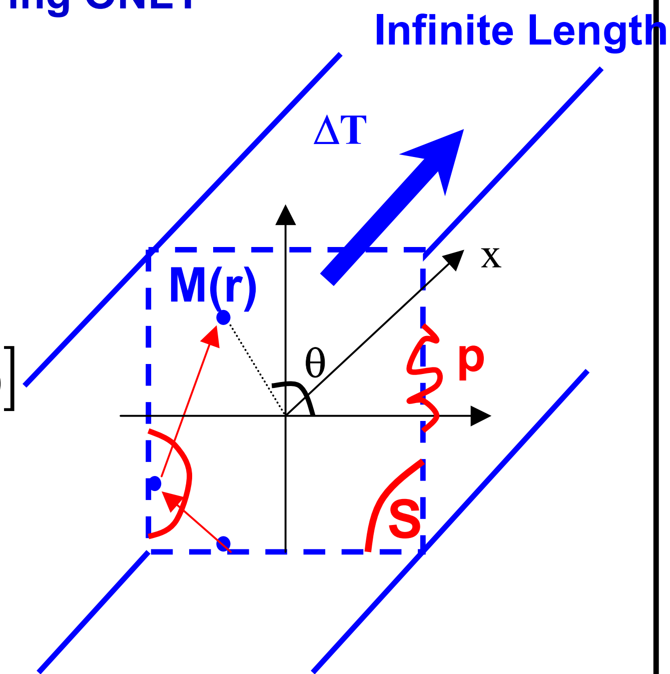




Free standing Bi Nanowire, M.S.Dresselhaus

BOLTZMANN TRANSPORT EQUATION

o 1D solution to BTE: Boundary Scattering ONLY



$$\cancel{\frac{\partial g(\nu)}{\partial t}} + \mathbf{v}.\mathbf{grad}\,g(\nu) = -\frac{g(\nu)}{\tau_{Bulk}}$$

$$g(\mathbf{r}) = \Lambda_{Bulk}.\cos\theta.\frac{\partial T}{\partial x}.\frac{\partial g_0}{\partial T}.[1-G(\mathbf{r},\mathrm{p})]$$

(Ziman -Electrons and Phonons)

$$\mathrm{q}(\mathbf{r})\mathrm{S} = \frac{1}{4\pi}\int_{4\pi}\int_{\nu=0}^{\nu_D} \mathrm{v}(\mu).\hbar\nu.\mathrm{g}(\mathbf{r}).\mathrm{D}(\nu).\mathrm{d}\nu.\mathrm{d}\Omega$$

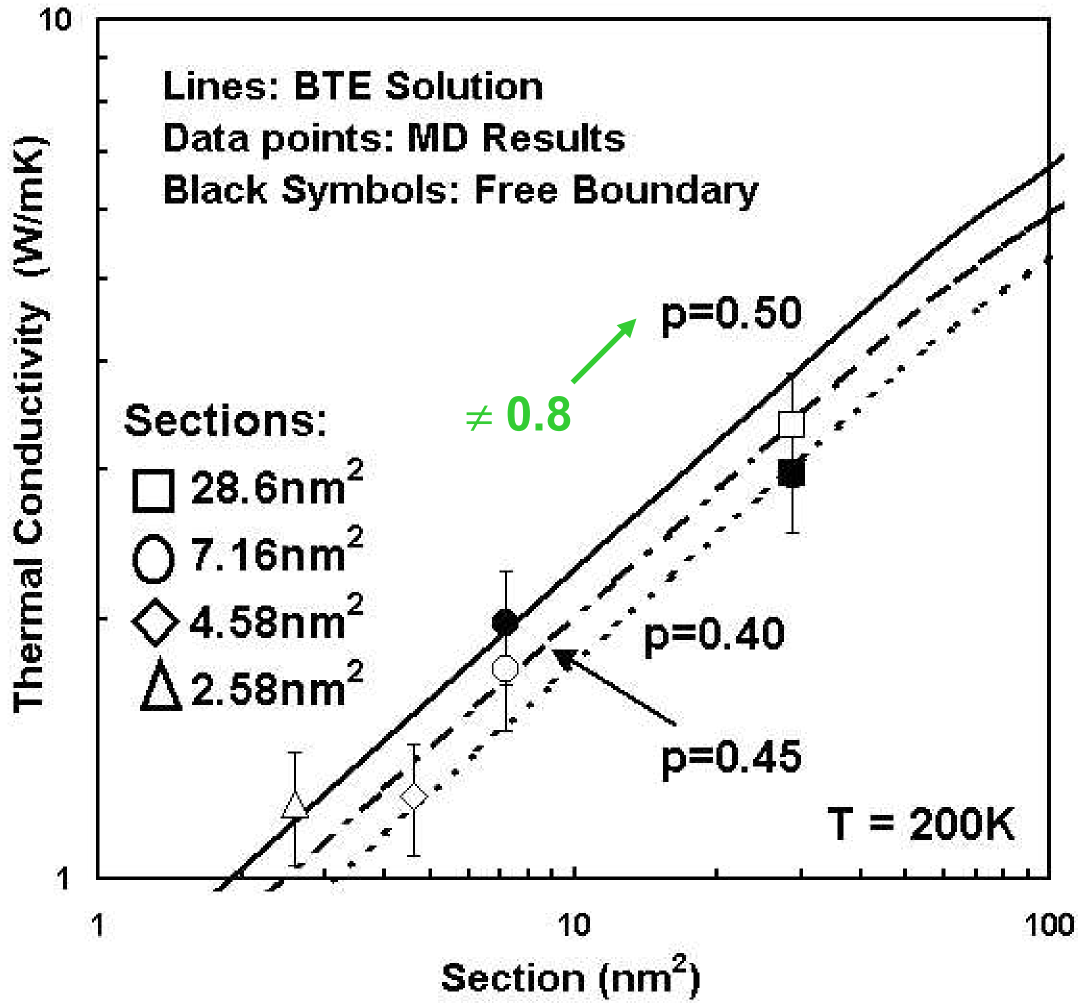
$$\boxed{\frac{\lambda_{nw}}{\lambda_{Bulk}} = \left(1-\frac{\Lambda_{Size}}{\Lambda_{Bulk}}\right)}$$

Function of G only

S. Volz and G. Chen, **Heat and Technology**, **18**, 37, 2000.

COMPARISON BETWEEN MD&BTE RESULTS

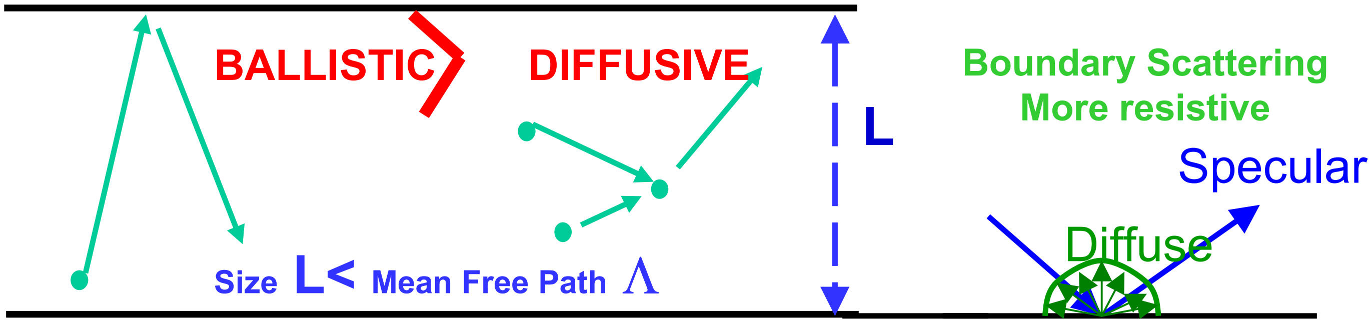
Is boundary scattering the only cause forthermal conductivity reduction?



S. Volz and G. Chen, **Applied Physics Letters**, **57**, 2056, 1999.

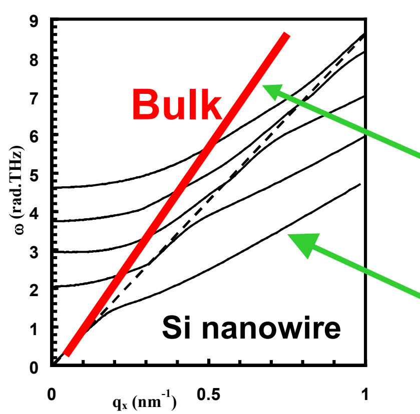
PHONON CONFINEMENT EFFECT ON HEAT CONDUCTION

- Ballistic Transport of Phonons



- Phonon Confinement

v_G and Λ Reduction



$$\frac{\partial^2 u}{\partial t^2} = v_t^2 . \nabla^2 u + \left(v_l^2 - v_t^2\right) \nabla (\nabla \bullet u)$$

$$\cancel{\vec{q} = -\lambda_{BULK} . \overrightarrow{grad\ T}}$$

$$\lambda_{effective} < \lambda_{BULK}$$

RPTE - THE DISCRETE ORDINATE METHOD

$$\Omega \mathbf{grad} L_\omega = \kappa_\omega \left(L_\omega^0 - L_\omega \right)$$

o S_8, discretizing in 48 directions (Ω, w_m) for finite length wire

Confinement effect

$$L_\omega = \sum_p \hbar\omega . g_\omega^p(r) . v_\omega^p(\Omega)$$

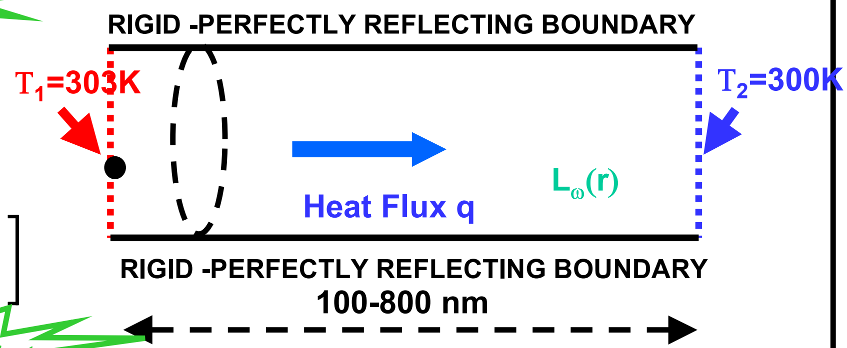
$$\Omega_m . \nabla L_{k,m} = \kappa_k \left[L_{k,m}^0 - L_{k,m} \right]$$

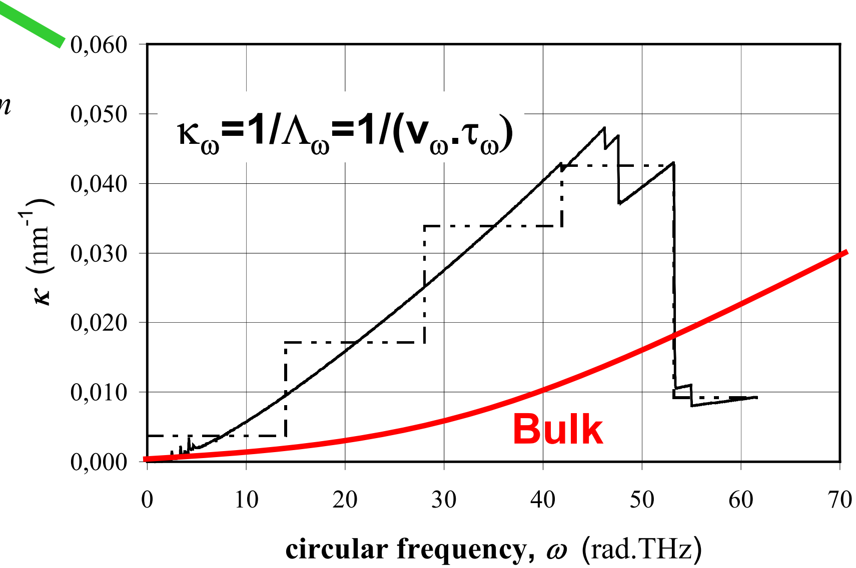
Confinement effect

$$q_{r,i,j} = \sum_{k=1,5} \sum_{m=1,48} w_m . L_{k,m,i,j} \Omega_m$$

$$\boxed{\lambda = \frac{q . L}{T_1 - T_2}}$$

T_{ij} ?





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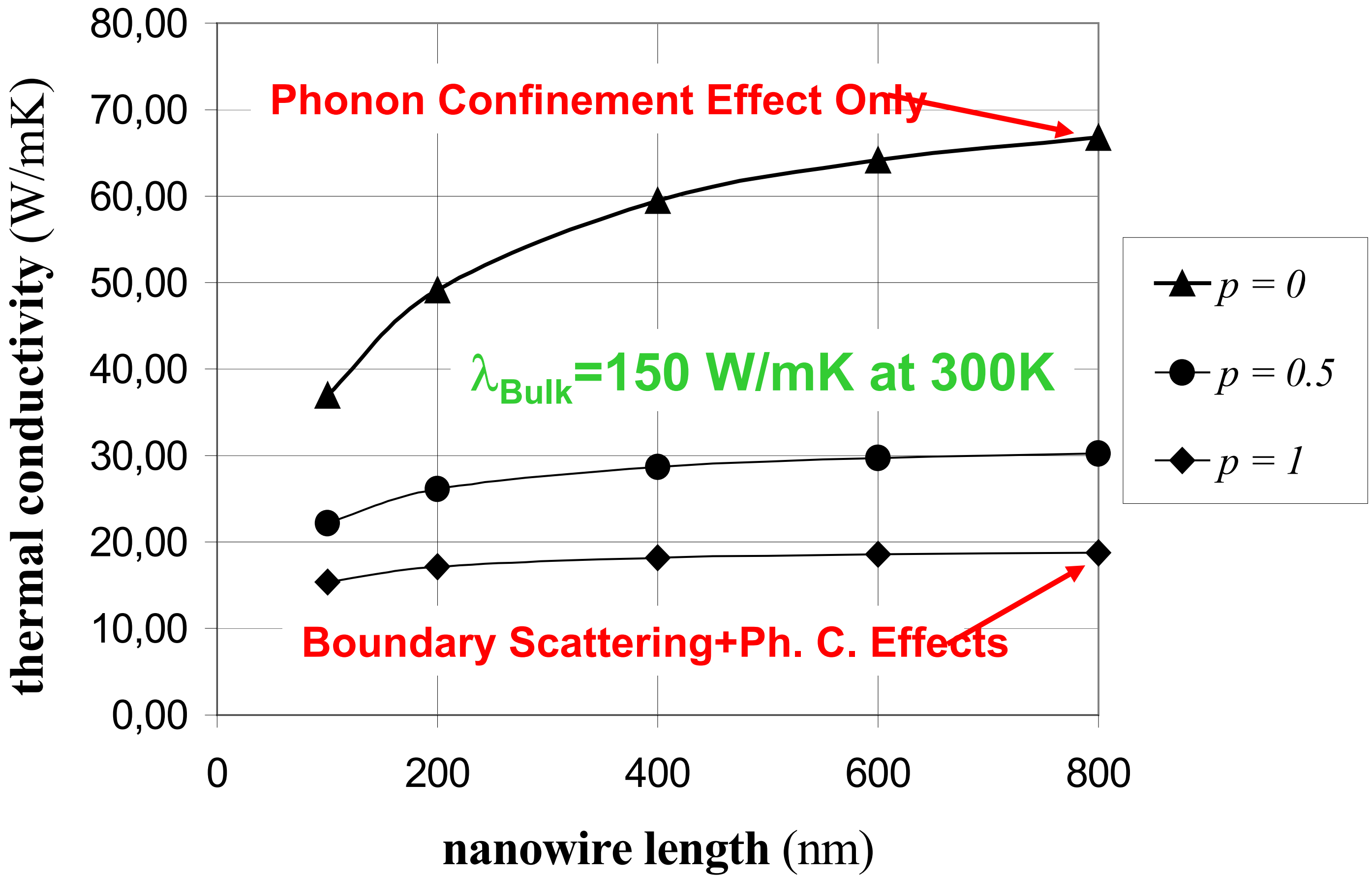
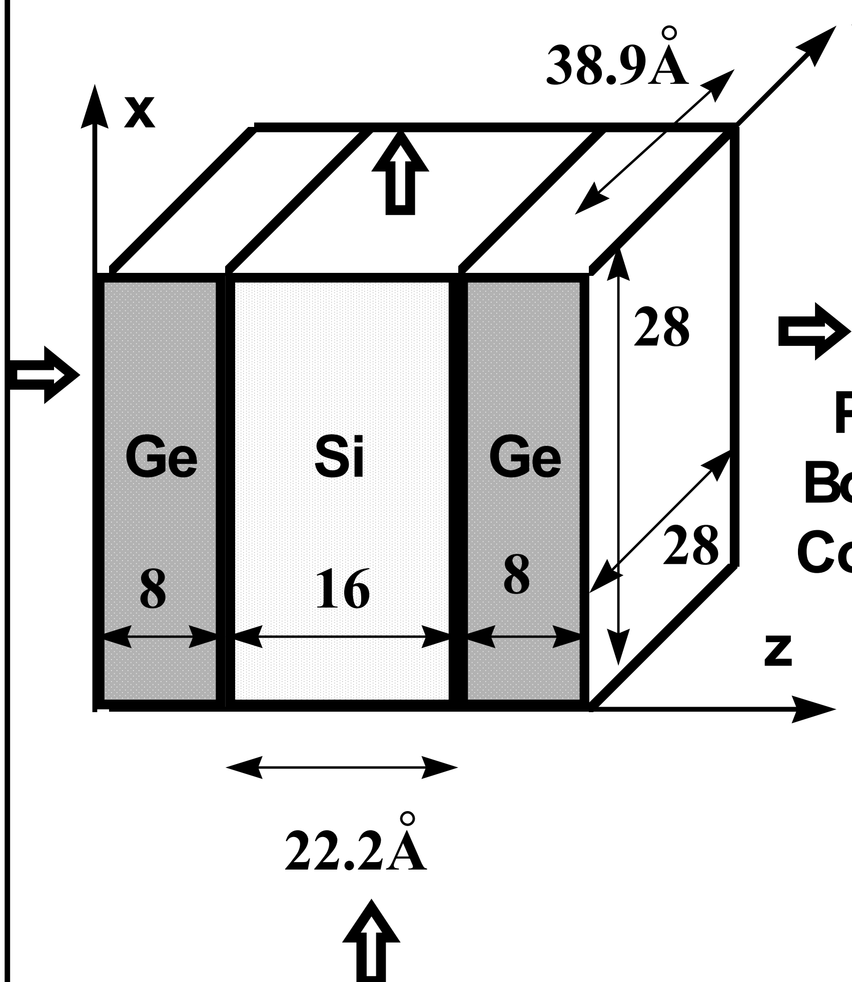
PHONON CONFINEMENT vs BOUNDARY SCATTERING



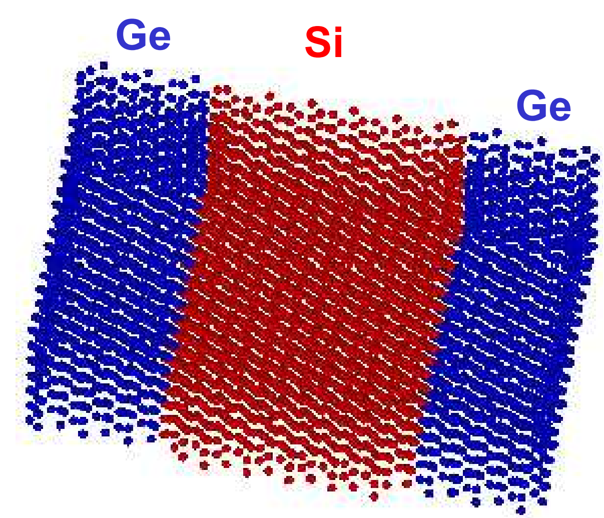
PHONON CONFINEMENT: 50% REDUCTION
BOUNDARY SCATTERING: 70% REDUCTION

S. Volz and D. Lemonnier, **Physics of Low-Dimensional Structures**, **5/6**, 91, 2000.

Si/Ge SUPERLATTICE MD MODELING

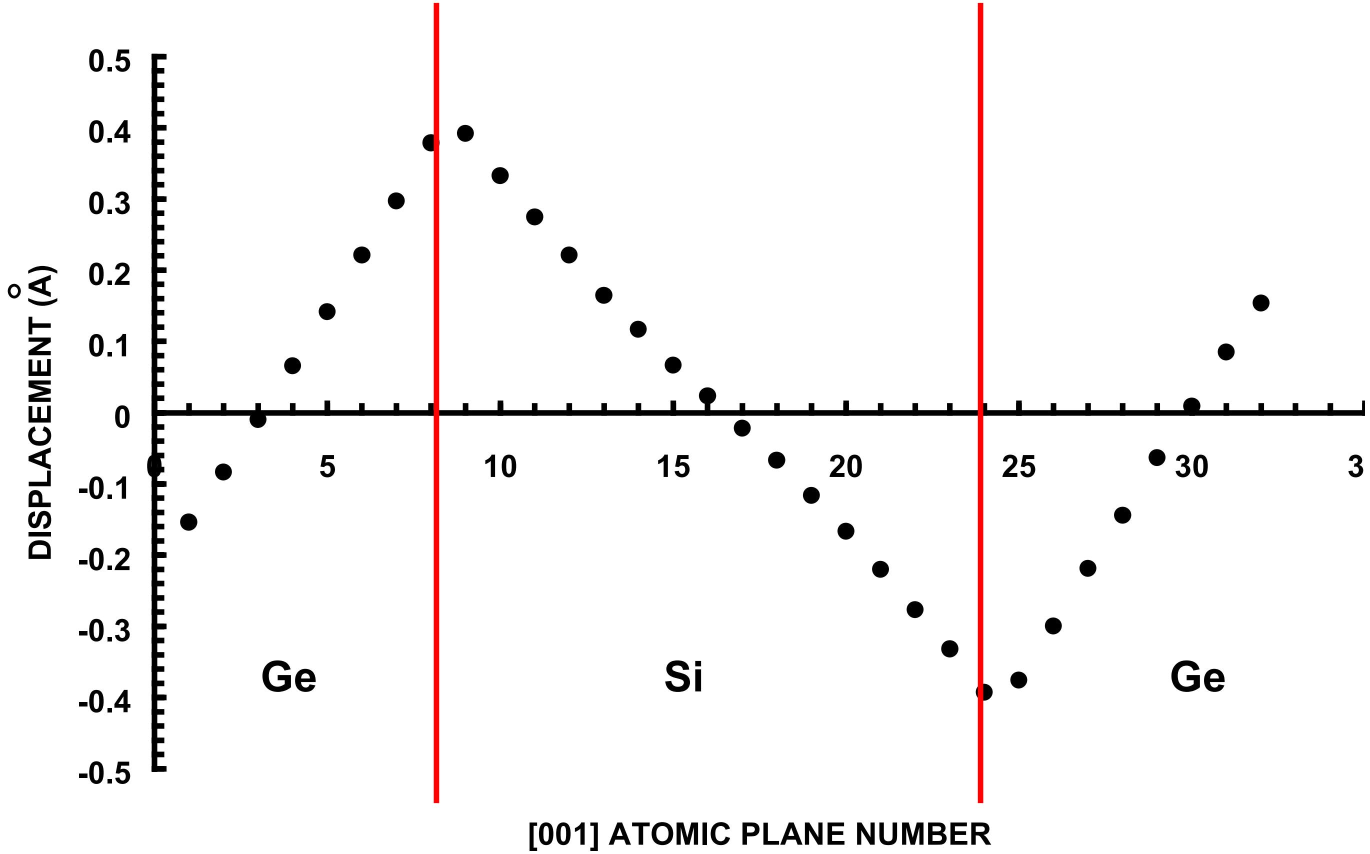


Periodic Boundary Conditions

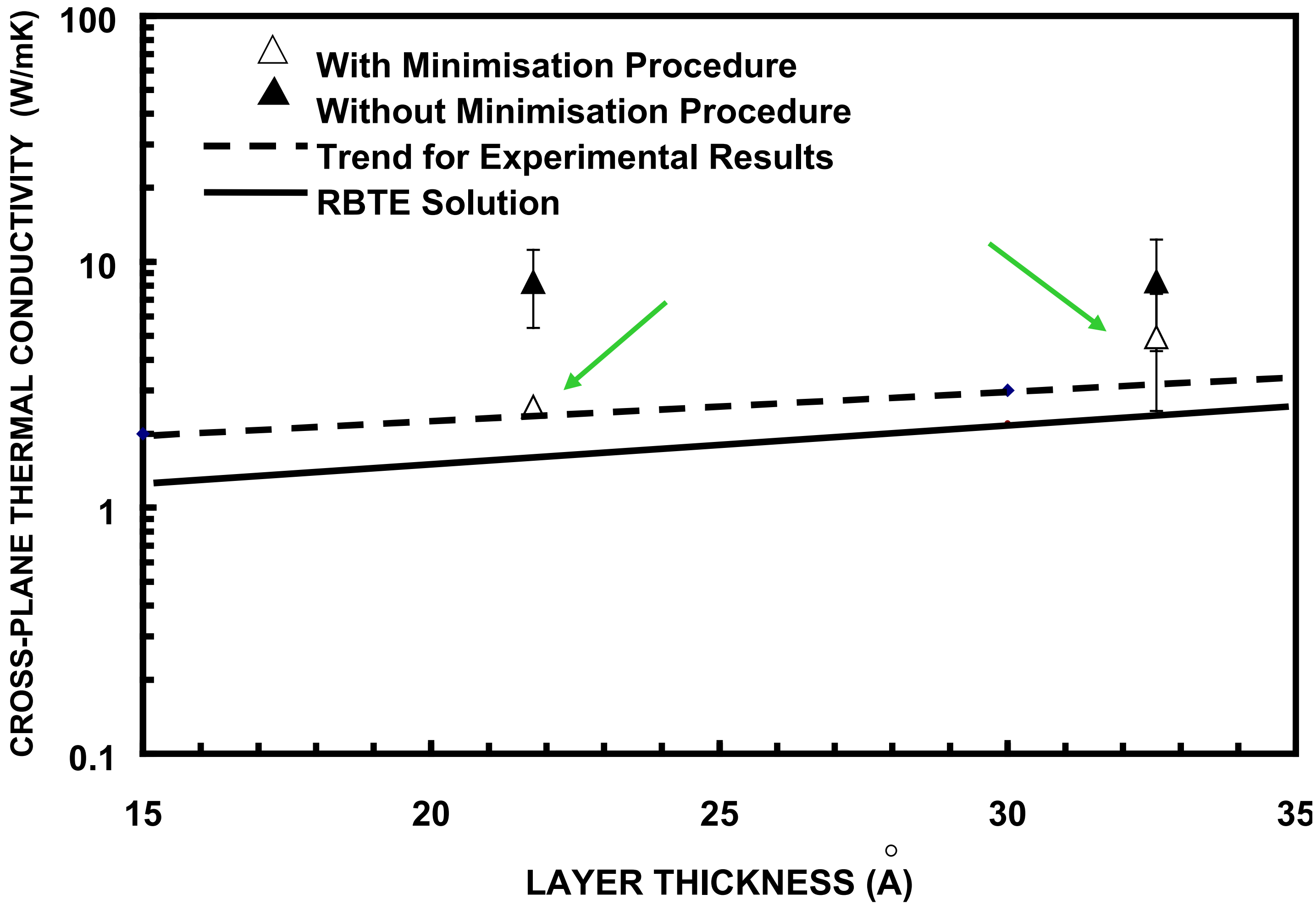


STRAIN EFFECT ON SUPERLATTICE STRUCTURE

- o Starting with mean lattice constant
- o Implementing Conjugate Gradient Method



SUPERLATTICE THERMAL CONDUCTIVITY



S. Volz, J.B Saulnier, G. Chen, P. Beauchamp, **Microelectronics Journal 31** (9-10) 815, 2000.

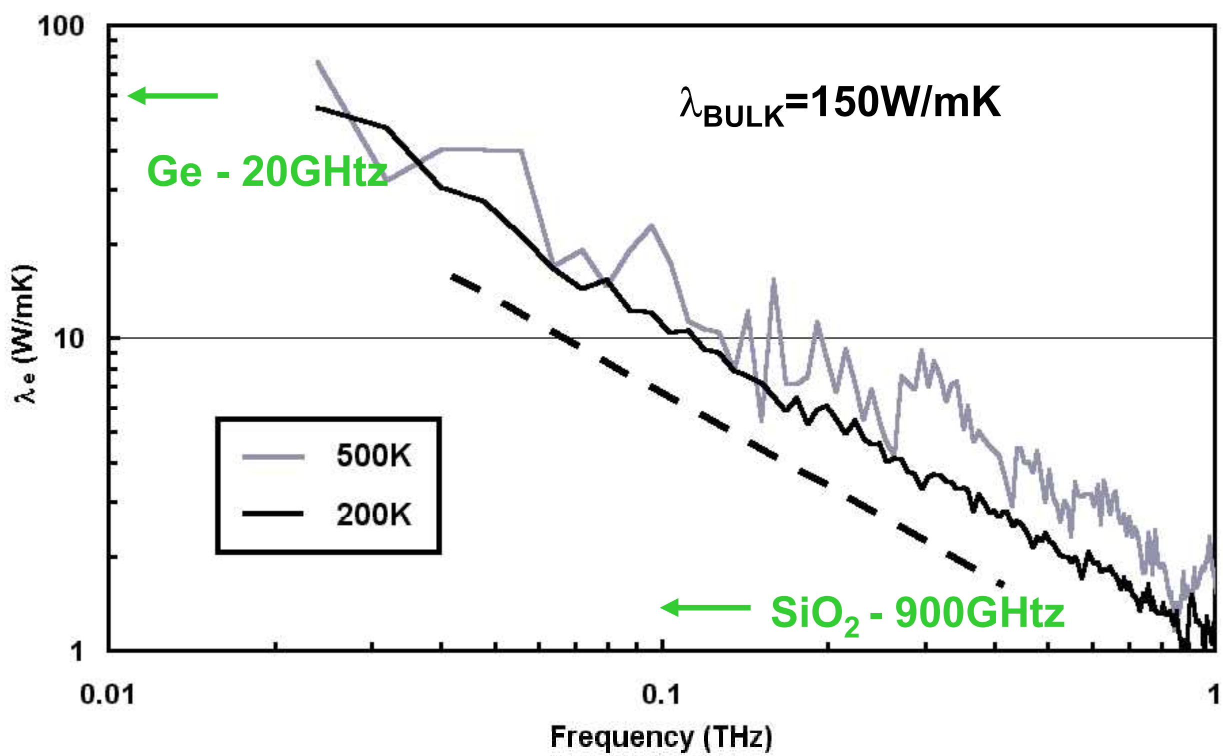
EFFECTIVE THERMAL CONDUCTIVITY AT GIGAHERTZ FREQUENCIES

o Fluctuation Dissipation Theorem

$$q(\omega) = \frac{V}{3.k_B.T^2}\int_0^{\infty}\langle q_0(0)\,q_0(t)\rangle e^{i\omega t}\,dt.\left\|\overrightarrow{gradT}\right\|$$

$$\boxed{\langle q_0(0)q_0(t)\rangle = \langle q_0(0)^2\rangle e^{-\frac{t}{\tau}}} \Rightarrow \boxed{\lambda_e = \frac{|q(\omega)|}{\left\|\overrightarrow{gradT}\right\|} = \frac{V}{3.k_B.T^2}.\frac{\langle q_0(0)^2\rangle}{\sqrt{1/\tau^2+\omega^2}}}$$

o ω^{-1} **dependence at Giga frequencies**



CONCLUSION

MOLECULAR DYNAMICS TECHNIQUE:

- o COMPLETELY DESCRIBES PHONON SCATTERING
- o ALLOWS THE SIMULATION OF DEFAULTS/STRAINS
- o GIVES ACCESS TO NON-EQUILIBRIUM REGIMES

- \- IS VERY HEAVY IN TERMS OF COMPUTATION TIME
- \- RELIES ON THE INTERACTION POTENTIAL VALIDITY
- \- DOES NOT INCLUDE QUANTUM EFFECTS

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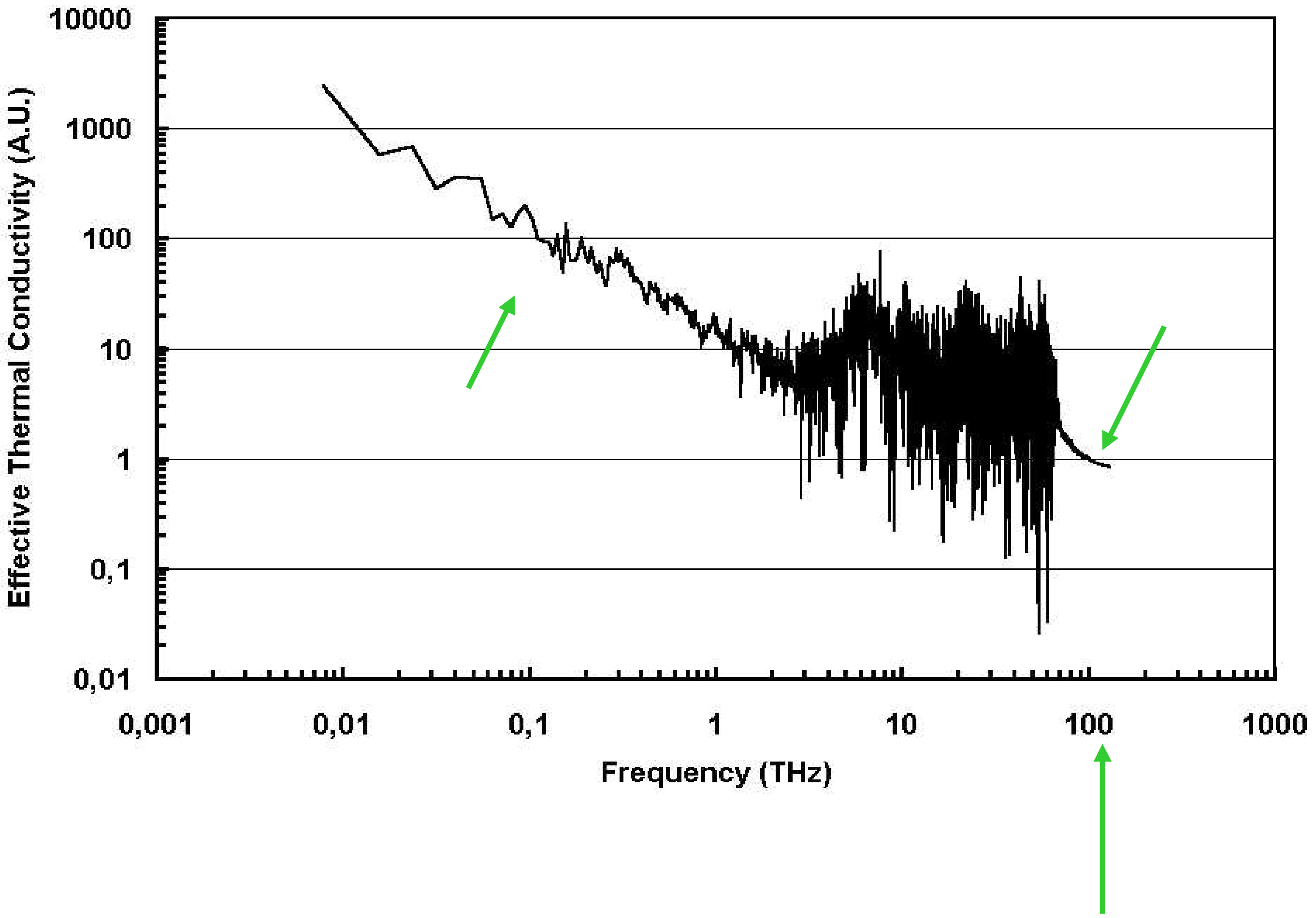
ULTRA SHORT TIME HEAT CONDUCTION



ω^{-1} LAW FOR Si THERMAL CONDUCTIVITY AT GIGAHTZ FREQUENCIES